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Publication date:
2019

Document Version
Publisher's PDF, also known as Version of record

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Multi-Scale Three-Dimensional Reconstruction of Ptychographic X-Ray Tomography Data

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Introduction

Ability to image volumetric structure of nano/microscale systems in material science brings a better understanding of the structure-function correlations that can significantly increase their performance in applied fields. Direct 3D reconstruction from coherent diffraction X-ray imaging (CDI) data requires large computational recourses. Therefore, we present here a multi-scale approach for reducing convergence time by fast reconstruction of low-resolution image and its further application as an input guess for high-resolution reconstruction.

Coherent X-ray diffraction imaging

In CDI experiment an incident wave interacts with a sample experiencing refraction and attenuation and propagates into a far-field detector that measures its intensity given by

$$I \cong \left| \mathcal{F}\left\{ P * \exp\left[\mathrm{i}k \int \mathbf{n} - \mathbf{1} \right] \right\} \right|^2$$

where P is illumination function, n is complex refractive index of the sample (object function) and $\mathcal{F}$ is Fourier transformation.

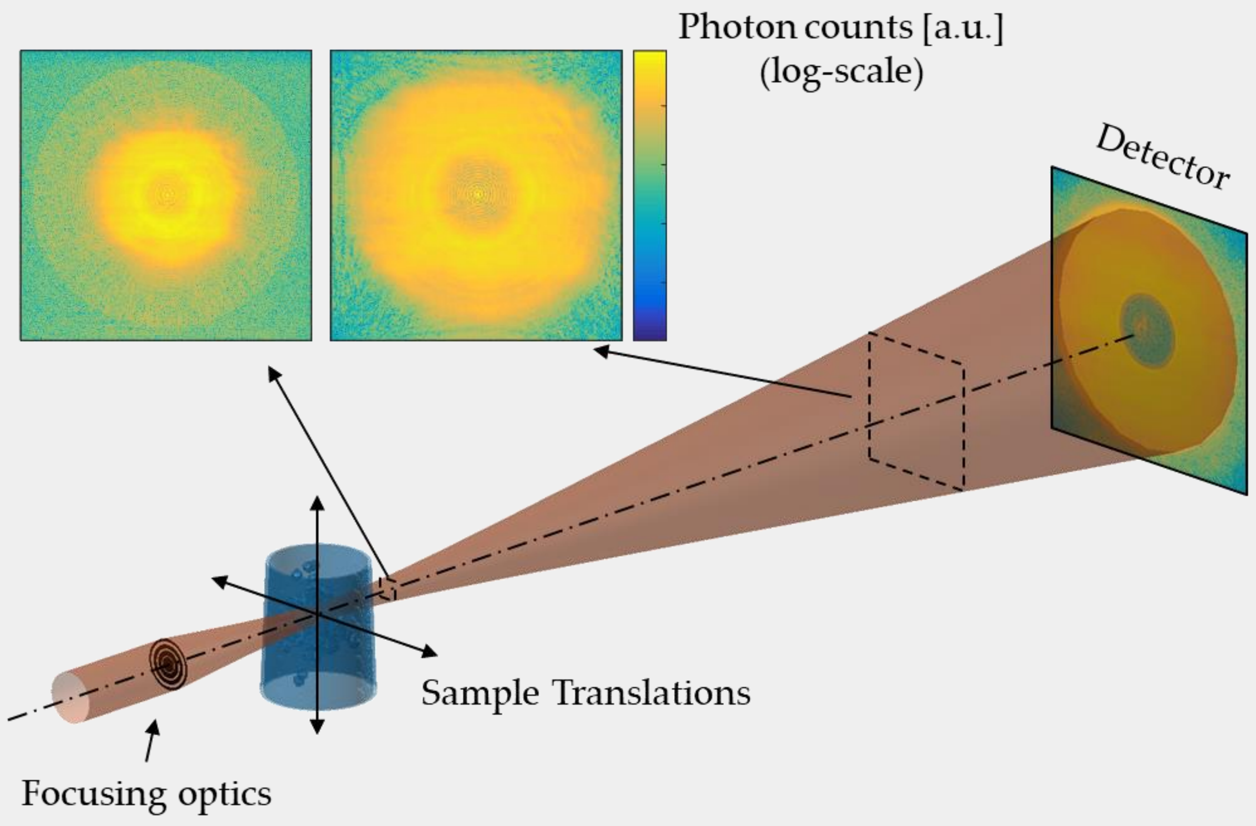

Figure 1: Schematic of ptychographic CDI.

Phase-retrieval algorithm

Reconstruction of the sample can be formulated as a least-squares optimization problem solved by iterative minimization of the difference between measured and approximated diffraction intensities:

$$\min_{\boldsymbol{x}} (I_j^a(\boldsymbol{x}) - I_j^m) \,.$$

Complex valued object function and squared modulus operation in the expression for intensity make the problem ill-posed and non-linear. Here, we use Levenberg-Marquardt algorithm (LMA) in combination with conjugate gradient method (CGM) to find the optimal solution.

Acknowledgments

This PhD project is part of the Marie Sklodowska-Curie Innovative Training Network MUMMERING (Multiscale, Multimodal, Multidimensional imaging for EngineeRING), funded through the EU research programme Horizon 2020.

Single-scale reconstruction

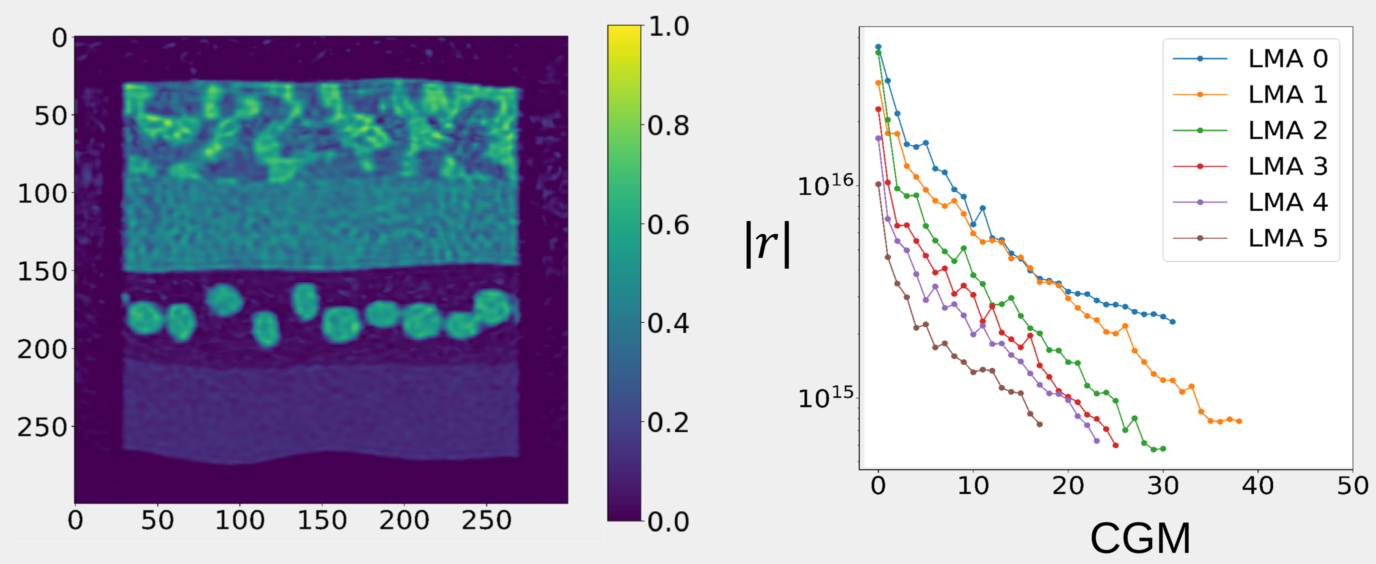

Figure 2: On the left, single-scale reconstruction from the complete diffraction data-set with zero-valued input is shown; on the right, residual values over LMA and CGM iterations are shown.

Low-resolution reconstruction

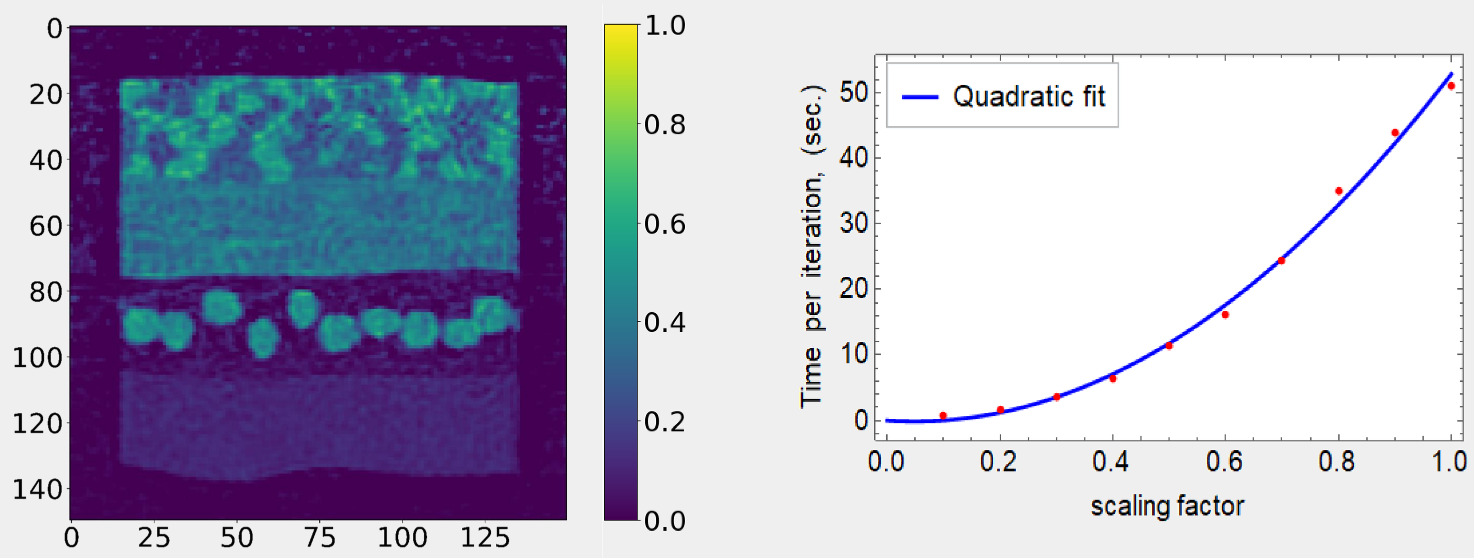

Figure 3: On the left, reconstruction from half of the diffraction data-set with zero-valued input is shown; on the right, processing time per iteration over scaling factor is shown.

Multi-scale reconstruction

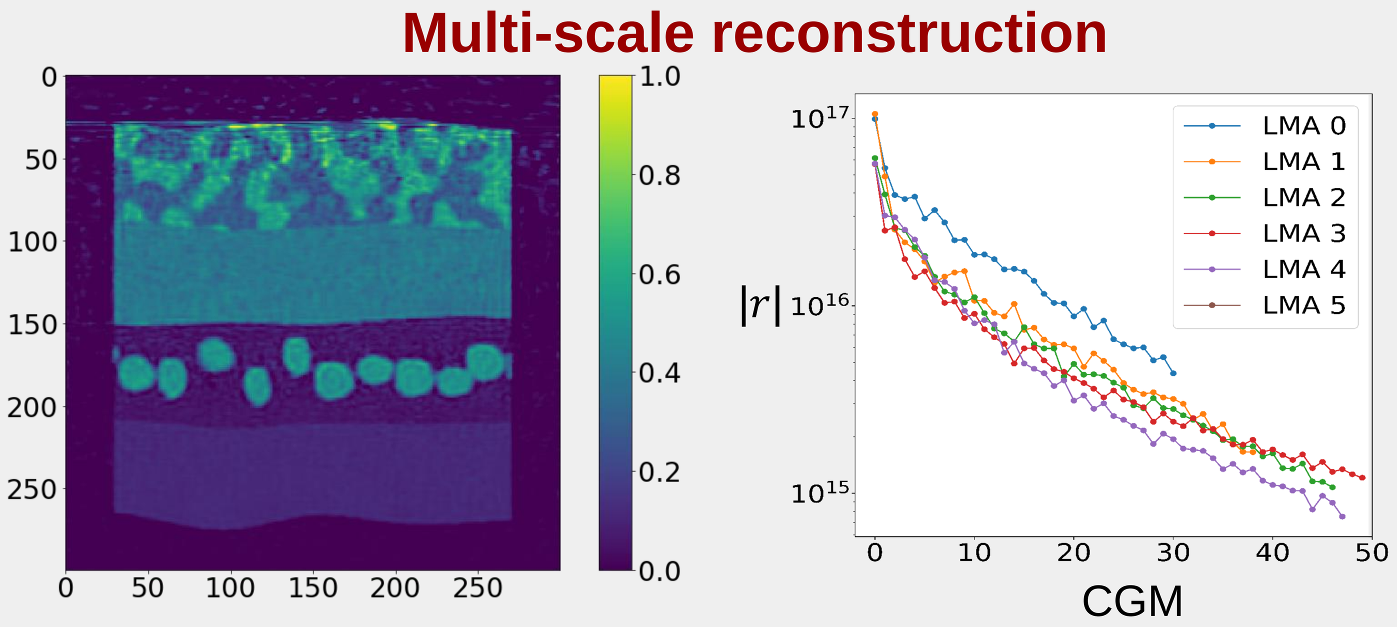

Figure 4: On the left, multi-scale reconstruction using a low-resolution image as an input; on the right: residual value over LMA and CGM iterations.

Future work

Here, we present an extension of the direct 3D ptychographic reconstruction using multi-scale approach. The next step towards decreasing computational costs of the algorithm is to solve the problem of scanning path optimization with instrumental constraints. The final goal is to implement developed algorithm to a real data.

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